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CRDEC-TR-88137

USING THEORETICAL DESCRIPTORS
IN STRUCTURAL ACTIVITY RELATIONSHIPS

II. POLARIZABILITY INDEX

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RESEARCH DIRECTORATE

September 1988

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<p>Quantitative structure activity relationships (QSAR) have been used successfully in the past to develop predictive equations for numerous biological and physicochemical properties. Kamlet and Taft used linear solvation energy relationships (LSER), a subset of QSAR, to correlate over 100 solute/solvent dependent interactions with a set of empirically derived descriptors. A major difficulty with this approach has been the use of these empirically determined parameters. A new approach based upon the generalized LSER approach has been developed. This technique, called Theoretical LSER, uses only structural and quantum chemically derived descriptors. The introduction of a new electronic term based upon polarizability will be described.</p>					
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PREFACE

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USING THEORETICAL DESCRIPTORS IN STRUCTURAL ACTIVITY RELATIONSHIPS

II. POLARIZABILITY INDEX

I. INTRODUCTION

In many areas of research and applications, it is necessary to know the physical and chemical properties of various chemical compounds. Often, many of the properties are either not known or not readily available. Therefore, property prediction methods must be developed in order to allow for reasonable estimation of the data gaps. Two compendia of estimation methods have been published.^{1,2}

The U.S. Army Chemical Research, Development and Engineering Center (CRDEC) has developed many of the physical/chemical property estimation methods in-house, because existing literature methods are not pertinent to CRDEC mission related compounds. For this reason, new models must be developed, or existing models modified to accept and adequately predict properties for these classes of compounds.

Quantitative Structure Activity Relationships (QSAR) have been used in the past to correlate structural and structure related descriptors and parameters to a variety of activities and properties.³⁻⁵ While the degree of correlation and the ultimate utility of the derived equation is dependent upon the basis set used, this technique can be used to predict useful properties *a priori*. QSAR, a subset of Linear Free Energy Relationships (LFER), assumes a linear form of the type:

$$\text{Log Activity} = \sum n_i a_i \quad (1)$$

The activity can be defined as potentially any physical/chemical/toxicological property. The terms n_i is the coefficient and a_i is the descriptor. The next paper in this series (Electronic Descriptors) gives a more in depth explanation of the relationship of QSAR to thermodynamics (unpublished data, July 1988).

1.1 Linear Solvation Energy Relationships

Linear Solvation Energy Relationships (LSER) have been shown to correlate very well with a wide variety of physical and chemical properties involving solute/solvent type interactions.^{3,6} LSER, as developed by Taft and Kamlet, takes the general form:

$$\begin{aligned} \text{Property} = & \text{Cavity Term} + \text{Polarizability Term} \\ & + \text{Hydrogen Bonding Terms} + \text{Intercept} \end{aligned} \quad (2)$$

In the LSER equation of interest to this study, the cavity term takes the form of the Molar Volume (V_m), that is, the size of the hole in the solvent matrix necessary for the solute to be solvated. The polarizability term (π^*) is a spectroscopically determined term, as are the hydrogen bonding terms (α and β). The Kamlet-Taft LSER parameters are all determined empirically; therefore, it is necessary to synthesize the compound. This, therefore, limits the use of LSER parameters in developing estimation methods, as the compound must first be synthesized and the LSER parameters measured.⁶

1.2 Theoretical LSER

The LSER correlations examined in the literature to date notes that the correlation coefficients are almost always above .98, with the standard errors on the order of about 5-6%. These would make ideal estimation routines were it not for the already mentioned empiricity of the LSER parameters. If the empirically derived descriptors could be replaced with corresponding computationally derived descriptors, then the utility for a priori prediction of physical/chemical properties would be greatly enhanced. This technical report is the second in a series describing this use of theoretical descriptors in LSER equations.⁷ In the first, the use of molecular volume (V_{mc}) in place of the molar volume is described and explained.

The introduction of nonempirical electronic terms has been traditionally unsatisfactory. Therefore, one or more new electronic descriptors must be developed and used in order for a successful incorporation into a completely theoretical LSER. Again, since the LSER results in previously mentioned high correlations, it can be used as the basis for any

substitutions. The electronic terms are therefore divided into two subsets: 1) a polarization term; and 2) hydrogen bonding terms. The hydrogen bonding terms are further divided into acidity (hydrogen bond donor) and basicity (hydrogen bond acceptor) terms. This paper will deal only with the development and incorporation into the Theoretical LSER of a polarizability term.

Quantum mechanics is often employed in order to obtain the most useful electronic descriptors.³ These descriptors have ranged from energy levels⁹ to electron densities and electrostatic potentials.^{10,11} In QSAR, these descriptors have typically given acceptable results, but the correlative fits have not approached those that have been obtained by the LSER.

The polarizability as generally accepted, is the distortion of a molecule when placed in an external electric field.⁶ The polarizability is therefore proportional to the strength of the induced dipole. Dewar and Stewart have included a the algorithm for the calculation of the polarization volume¹² in their latest release of MOPAC.¹³ One difficulty immediately observed was the dependency of the polarization volume on the size (volume) of the molecule. Since the polarization volume is proportional to volume, dividing by the molecular volume should remove the size dependency for the electronic characteristics. This resulting Polarizability Index (π_1) should have little or no correlation to molecular volume, as well as constitute a reasonable electronic descriptor. This paper will describe the use and the chemical applicability of the Polarizability Index to developing a theoretical LSER with the emphasis on physical property prediction. A comparison of the theoretical LSER to the corresponding LSER using the solvatochromic parameters will also be made.

2. EXPERIMENTAL PROCEDURES

2.1 Theoretical and Calculated Parameters

All geometries were optimized using the MNDO algorithm incorporated in the MOPAC series of molecular orbital programs.¹³ The molecular volumes were generated from the MNDO optimized geometries using the method of Hopfinger,¹⁴ incorporated in the Chemometric and Biometric Modeling (CBM) Branch's Molecular Modeling Analysis and Display System (MMADS).¹⁵

All calculations were performed on a microVAX II running the VMS operating system.

2.2 LSER Parameters

All π^* and β terms and the activities were taken from selected papers of Kamlet, Taft and co-workers.¹⁶⁻¹⁸

2.3 Experimental Data

The activities used for the correlations in this study were taken from several papers in several different fields. The Octanol/Water Partition Coefficients were taken from data compiled by Kamlet and Taft.¹⁶ The Fish Toxicity data was taken from a report by Konnemann involving LC₅₀ experiments on guppies (*Poecilia Reticulata*) using 50 industrial pollutants.¹⁷ The Charcoal Adsorbitivity were obtained from papers by Abe¹⁹ and Giusti.²⁰

All multiple linear regressions were performed using HASSLE-STAT, running on a microVAXII. All plots were made on a Hewlett-Packard 9845B microcomputer using a graphics package written by L. M. Sturdivan, CRDEC.

3. RESULTS

Throughout the equations listed below, the molecular volume, polarizability index, solvatochromic parameters and activities have the following abbreviations:

LOG Kow	= Log (Octanol/Water Partition Coefficient)
α	= Charcoal Adsorbitivity
LC ₅₀	= 50% Lethal Concentration (mg/kg)
V _{mc}	= Molecular Volume (Å ³)
V _m	= Molar Volume (ml/mol)
π_1	= Polarizability Index
π^*	= Solvatochromic Polarizability Term
β	= Solvatochromic Hydrogen Bond Basicity Term

For the particular systems of interest, the LSER equation takes the form of equation 3:

$$\text{LOG Activity} = mV_m + p\pi^* + b\beta + A_0 \quad (3)$$

The terms m , p , and b are the coefficients of regression for the corresponding variable (V_{mc} , π^* , and β , respectively), and A_0 is the intercept. Any activity, therefore, is dependent upon a) the size of the substrate molecule, b) the ability of a dipole moment to be induced by polarization of the electron cloud, and c) the relative ability to act as a hydrogen bonding base (acceptor). The Theoretical LSER parameters replace on a one for one basis directly into equation 3, with the already mentioned difference being that these parameters are not empirically measured but calculated entities. The Theoretical LSER with the associated parameters is shown in equation 4:

$$\text{LOG Activity} = mV_{mc} + p\pi_I + b\beta + A_0 \quad (4)$$

3.1 Polarizability Index

3.1.1 Description of π_I

The polarizability is defined by the equation:

$$\Delta W = \alpha E^2 \quad (5)$$

where:

ΔW = Change in Molecular Energy due to Electric Field

α = Polarizability (\AA^3)

E = Strength of Electric Field (V/\AA^2)

The polarizability, α , is given in units of volume, typically cm^3 or \AA^3 . Using this basic equation, with modifications of Dewar and Stewart, it is possible to calculate the amount of deformation due to a constant electric field. MOPAC uses an electric field of .0696 V/\AA .

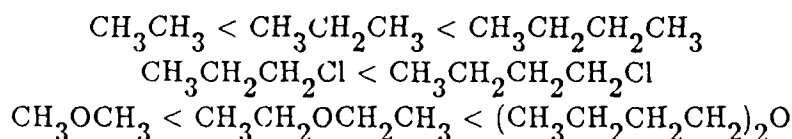
A primary consideration in the development of theoretical LSER parameters and descriptors is the descriptors must make chemical sense. That is, the descriptor must explain some interaction/property such that the phenomenon agrees with chemical

intuition. There are numerous examples of descriptors and models in the literature that are excellent fits, but the models themselves make no chemical sense.^{21,22} Therefore, as a first step prior to incorporating the Polarizability Index (π_I) into LSER equations, the π_I must be examined for chemical content.

Table 1 lists the name, internal identification number of the compounds examined in this study, molecular volume, and the Polarizability Index. The table is ordered by increasing π_I . As noted above, the units of the polarizability from MOPAC was \AA^3 , a measure of units. In principle, if one were to divide the polarizability by the molecular volume, also in terms of \AA^3 , the resulting number, π_I , would be unitless, and would therefore be independent of molecular size. The correlation of π_I and the Molecular Volume for the compounds in Table 1 is .184, which indicates no dependency upon volume in the Polarizability Index. A similar correlation with the corresponding Polarization Volume (not shown) and molecular volume is .90. From a purely statistical view, the Polarizability Index and molecular volume have no codependence and may be used in conjunction with V_{mc} in multiple linear regressions.

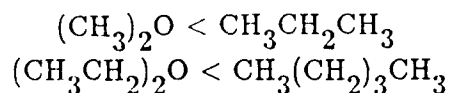
3.1.2 Trends of the Polarizability Index

Several chemically intuitive trends are apparent from the data listed in Table 1. First, smaller molecules have a smaller π_I than larger molecules of the same class. As examples:

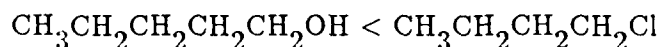
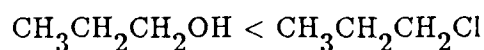


This is in agreement with what is expected, smaller molecules have a fewer number of electrons that are able to move, thus giving rise to a smaller polarizability.

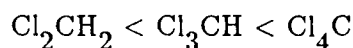
Second, molecules with highly electronegative atoms (like oxygen and nitrogen) have lower π_I than the corresponding alkane. For instance:



The higher electronegative compounds will bind the electrons tighter, preventing deformation of the electron cloud. Along this same line, chlorine, which is larger than the second row elements, has a greater number of electrons. Therefore, chlorine would be expected to have a larger π_1 than analogous compounds containing carbon, oxygen, or nitrogen. This can be seen in two examples:

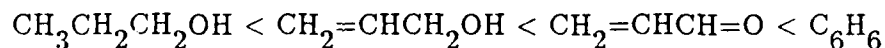


In adding chlorines, one would expect to observe the π_1 increase dramatically across the series. Indeed, this is the case as:



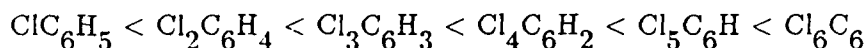
This can be easily explained as the dramatic increase in loosely held electrons, increases the ease in which they could be moved about.

As unsaturation is increased, chemical intuition tells us that the degree of polarizability will markedly increase. The π_1 predicts this trend, from no unsaturation, to one double bond to two double bonds to aromatic:



The aromatics, which have the most easily polarizable electron cloud, have the highest π_1 values, at .1200 or above. Within the aromatics, it can be seen that adding more polarizable groups result in the increase of the π_1 value.

Adding chlorines to the benzene ring has a similar effect as to that described above. One would expect to observe a systematic increase in the polarizability, and indeed this is seen with π_1 , where:



This list is by no means complete, and additional compounds and trends must be examined, especially in existing series. A technical report describing π_1 in depth and examining the relationship to easily rationalizable chemical phenomena is being prepared.

3.2 Polarizability Index in LSER

The applicability of the π_1 is not so much in explaining intuition as has already been seen, but in replacing the polarizability term of the LSER. Three example activities have been examined, partition coefficients, toxicity, and charcoal adsorbitivity. For each activity, a comparison of the LSER versus the theoretical LSER has been made. In order for a better comparison of the π_1 term with the π^* term, the molecular volume is used in the LSER equations as well as the Theoretical LSER equations. The hydrogen bonding term β is also used in both equations.

3.2.1 Octanol/Water Partition Coefficient

The Octanol/Water Coefficient has been used extensively in QSAR and in medicinal and toxicological chemistry as a excellent system for modeling the transport properties of chemical compounds. Examples of the use of this model are numerous in the literature, usually dealing with predicting toxicities. Because of the importance of this partition coefficient, data is very prevalent in the literature. Also, if it is possible to successfully model the Kow, then it also stands to reason that the activities for which it is a good model would also be modeled well.

Following the logic of Kamlet and Taft, the first attempt at a correlation should encompass a reasonably limited, well behaved data set. For this purpose, a series of aliphatic compounds were chosen. Equations 6 and 7 show the relationships obtained from the use of π_1 and π^* , respectfully.

$$\text{LOG Kow} = 3.281(V_{mc}/100) - 1.741(\pi_1^{**}10) - 4.573\beta + 1.772 \quad (6)$$

$$N=36 \quad R=.9722 \quad \text{SEE}=.3208$$

$$\text{LOG Kow} = 2.569(V_{mc}/100) - 1.216(\pi^*) - 3.492(\beta) + .721 \quad (7)$$

$$N=36 \quad R=.9908 \quad \text{SEE}=.1855$$

The volume term, V_{mc} , was divided by 100 and the polarizability index, π_1 , was multiplied by 10 in order to have approximately the same ranges for each of the parameters. The data for the compounds used, as well as the predicted values and residuals for equations 6 and 7 are found in Tables 3 and 4, respectively. Figure 1 displays a plot of the predicted LOG Kow versus the experimental value for equation 6. The line represents a "perfect" fit. The deviation from the line (which has a slope of 1.00 and an intercept of 0.00) represents the residuals. Figure 2 is an analogous plot for equation 7.

The signs of the coefficients of each of the two equations correspond to expected trends. Because water hydrogen bonds to itself better than octanol, it should require a larger energy to create a cavity for the solute to fit. Larger compounds, requiring larger cavities be created, should partition preferentially into the octanol layer, giving rise to a positive coefficient for this parameter. On the other hand, a highly charged species or one that has a high affinity for hydrogen bonding will partition into the water layer preferentially, giving rise to a negative coefficient for this parameter. A compound with a high polarizability would signify a great likelihood for an induced dipole type interaction. Since water has a greater dipole moment than octanol (calculated from MNDO: for water $\mu = 1.783$ and for octanol $\mu = 1.504$), the compounds with larger polarizabilities should partition into the water layer preferentially, giving rise to a negative coefficient for π^* and π_1 .

The size for the coefficients for each of the parameters in equations 6 and 7 are roughly equivalent, with β being the most significant, followed by V_{mc} , and then by either

π_1 or π^* . From the correlation coefficient (R), and the standard error of the estimate (SEE), it is easily seen that the LSER parameters create a better correlative model for this data set by a significant margin (almost a factor of two).

However, as one adds nonstandard (i.e., compounds that Taft and Kamlet found did not obey the LSER ground rules), one sees that the theoretical LSER equation (equation 8) is not reduced in correlative ability, but actually improves in both R and SEE marginally. On the other hand, the LSER equation (equation 9) is reduced marginally in effectiveness.

$$\text{LOG Kow} = 3.285(V_{mc}/100) - 1.2377(\pi_1 * 10) - 4.596\beta + 1.240 \quad (8)$$

$$N=51 \quad R=.9744 \quad SEE=.2762$$

$$\text{LOGKow} = 2.768(V_{mc}/100) - 1.2377(\pi^* * 10) - 3.703\beta + .183 \quad (9)$$

$$N=51 \quad R=.9889 \quad SEE=.1825$$

In examining the coefficients and the effects of adding the alcohols on the coefficients, the theoretical LSER coefficients change very little, with the π_1 being the only descriptor to vary by more than 0.1. On the other hand, the LSER descriptors all change by at least .1 except the π^* . This indicates that modifications due inherent in alcohols are all electronic in nature, and that π_1 adequately contains all of the information for this difference. On the other hand, π^* does not change, indicating that it does not adequately incorporate the electronic differences between aliphatics and aromatics. This can be seen further in the the steric term V_{mc} and the electrostatic charge term β do change dramatically in the LSER equation, but not in the theoretical equation. This also indicates some cross correlation between the LSER descriptors, especially π and β and π^* and V_{mc} , but not between the theoretical LSER descriptors. Table 5 contains the

theoretical LSER parameters, LOG Kow observed, the LOG Kow, and residuals as predicted by equation 8. Table 6 contains the same information for the LSER parameters and predicted results and residual based upon equation 9.

The single largest class of compounds that the LSER equation has had difficulties with in the past has been the aromatics.⁶ Kamlet and Taft, in order to ensure good correlations, have added a correction factor of 10 cm³/mol to the molar volume (and hence, to the molecular volume). They have explained this in terms of the planarity of the benzene ring, and the fact that in solution the phenyl group is planar and actually has a greater volume depending on the particular orientation. Equations 10 and 11 show the theoretical LSER and LSER, respectively for aliphatics, alcohols, and aromatic compounds, without the 9.5 cm³/mol correction to the V_{mc}. Table 7 show the Theoretical LSER parameters, observed, predicted Kows, and residuals for equation 10. Table 8 displays the same for the LSER parameters and equation 11.

$$\text{LOGKow} = 3.176(V_{mc}/100) - 1.110(\pi^*_I \cdot 10) - 4.512\beta + 1.179 \quad (10)$$

$$N=69 \quad R=.9756 \quad \text{SEE}=.2675$$

$$\text{LOGKow} = 2.970(V_{mc}/100) - 0.667(\pi^* \cdot 10) - 4.030\beta + .342 \quad (11)$$

$$N=69 \quad R=.9838 \quad \text{SEE}=.2189$$

The addition of the aromatics has further reduced the correlation coefficient and increased the standard error of the estimate of the equation using the LSER parameters. The coefficients for equation 10 do not change dramatically with the addition of the new class of compounds. The LSER based π^* does change dramatically, thereby forcing minor but noticeable changes in the other two descriptors. This further indicates the robustness and stability of the theoretical LSER parameters.

Figures 3 and 4 give a general pictorial view of all of this. Figure 3 shows predicted LOG Kow versus the experimental KOW for all of the compounds in Table 7. Figure 4 shows the same from Table 8. As in Figures 1 and 2, the line represents a "perfect fit", that is, the experimental and the predicted have the same value.

3.2.2 Charcoal Adsorbitivity

Another type of solubility is the distribution of a solute between a solvent and a solid adsorbent. An example of this is the adsorption of organic nonelectrolytes onto activated carbon from aqueous solutions. The property considered is α , and is defined in equation 12:

$$\alpha = \lim_{C \rightarrow 0} \frac{X}{C} \quad (12)$$

where C is the equilibrium concentration and X is the amount of the compound adsorbed on the carbon. The quantity α , then, represents the partition coefficient between the solution and solid phases at infinite dilution. Kamlet and Taft have reported LSER regressions on 37 of the compounds examined by Abe and Giusti.^{19,20} The computational methods for calculating V_{mc} and π_1 was not capable of handling four of the compounds. The resulting theoretical LSER and LSER are found in equation 13 and 14.

$$\text{LOG } \alpha = 2.653(V_{mc}/100) + 0.287(\pi_1 * 10) - 2.603\beta - 1.599 \quad (13)$$

$$N=33 \quad R=.9487 \quad \text{SEE}=.2532$$

$$\text{LOG } \alpha = 2.970(V_{mc}/100) + 0.739(\pi^* * 10) - 2.312\beta - 1.929 \quad (14)$$

$$N=33 \quad R=.9557 \quad \text{SEE}=.2357$$

The resulting equations are very similar; the term in each of the equations is in actuality statistically not significant and has much less impact on the correlation than either the V_{mc} or β terms. Table 9 gives the theoretical LSER parameters, observed and

predicted LOG α and the residuals based upon equation 13. Table 10 lists equivalent results for the LSER parameters, based upon equation 14. Table 9 is graphically displayed in Figure 5, with the aromatics and alcohols separated into two subgroups, plotted with different symbols. Figure 6 displays the same for Table 10.

This would mean that the adsorption on charcoal, as measured in terms of partitioning from an aqueous layer, depends highly upon the size of the solute and the hydrogen bonding capability, and relatively little upon the polarizability of the electron cloud, or the dipole-dipole interaction. Furthermore, the coefficient of V_{mc} is positive, signifying that larger compounds will preferentially be adsorbed onto the charcoal. This is to be expected for the same reasons as given above, the energy required to create a cavity in water is fairly high. The hydrogen bonding term is negative, meaning that the better the base, the more it will prefer to stay in the aqueous phase. This is also the same as above, in that more electrostatic interaction will stabilize a solute-solvent pair.

3.2.3 Konnemann's Fish Toxicity

A third type of solvent solute interaction, and a completely different application of the theoretical LSER and the LSER, is to toxicity and biological activity. A very common descriptor for QSAR equations and relationships has been the octanol/water partition coefficient.²³ This is primarily due to the perception that the transport to the active site of the chemical compound is necessary and is often the limiting step. Since this is primarily a partitioning between hydrophilic and lipophilic regions, an appropriate partition coefficient would model this transport well. Hansch and Leo have found that the octanol/water partition coefficient models the transport behavior.²⁴ As has been shown above, both the theoretical LSER and LSER correlate very well with the LOG Kow. Therefore, the LSER and the theoretical LSER should also correlate highly with toxicity. Taft and Kamlet (unpublished data on the fat head minnow and the guppy, July 1988) have reported several studies where the LSER does correlate well with a variety of toxicity measures.

Konnemann measured the LC_{50} of 24 aliphatic and aromatic compounds on guppies (*Poecilia Reticulata*). The resultant multiple linear regressions for the theoretical LSER and LSER are found in equations 15 and 16. Table 11 lists the parameters, observed and predicted results, and residuals associated with equation 15. Figure 7 shows this pictorially. Table 12 and Figure 8 show analogous results for equation 16.

$$\text{LOG LC}_{50} = -3.061(V_{mc}/100) - 0.550(\pi_I \cdot 10) + 3.279\beta + 5.971 \quad (14)$$

$$N=24 \quad R=.9802 \quad \text{SEE}=0.2972$$

$$\text{LOG LC}_{50} = -3.157(V_{mc}/100) - 0.003(\pi^*) + 3.277\beta + 5.397 \quad (15)$$

$$N=24 \quad R=.9778 \quad \text{SEE}=.3152$$

As can be seen from equations 14 and 15, the toxicity is predicted to be higher with larger compounds (that is, a smaller LC_{50} signifies a more toxic compound). In addition, the better the solute is as a hydrogen bond base (better electrostatic interactions) the higher LC_{50} and the lower the toxicity. The polarizability term is completely insignificant in the LSER equation, and while the π_I is statistically not significant, it does have a minor effect in the theoretical LSER.

4. CONCLUSION

This study reported a new electronic measure for incorporation into QSAR equations. This measure, π_I , while it does not correlate with Taft and Kamlet's π^* , does replace it adequately in LSER equations. Combined with the molecular volume, a powerful series of theoretically based descriptors is being developed based upon the LSER approach. These theoretically derived descriptors once completely developed, will permit the *a priori* determination of selected physical properties once the theoretical LSER has been developed.

In several of the LSER parameters, Kamlet and Taft have found that correction factors need to be applied to certain classes of compound in order to "bring them in line" with the other compounds. These include a correction to the π^* for chlorinated compounds and a correction to molar volume for both alcohols and aromatics. The theoretical LSER has not incorporated any such correction terms to date, although such may be necessary at some future point.

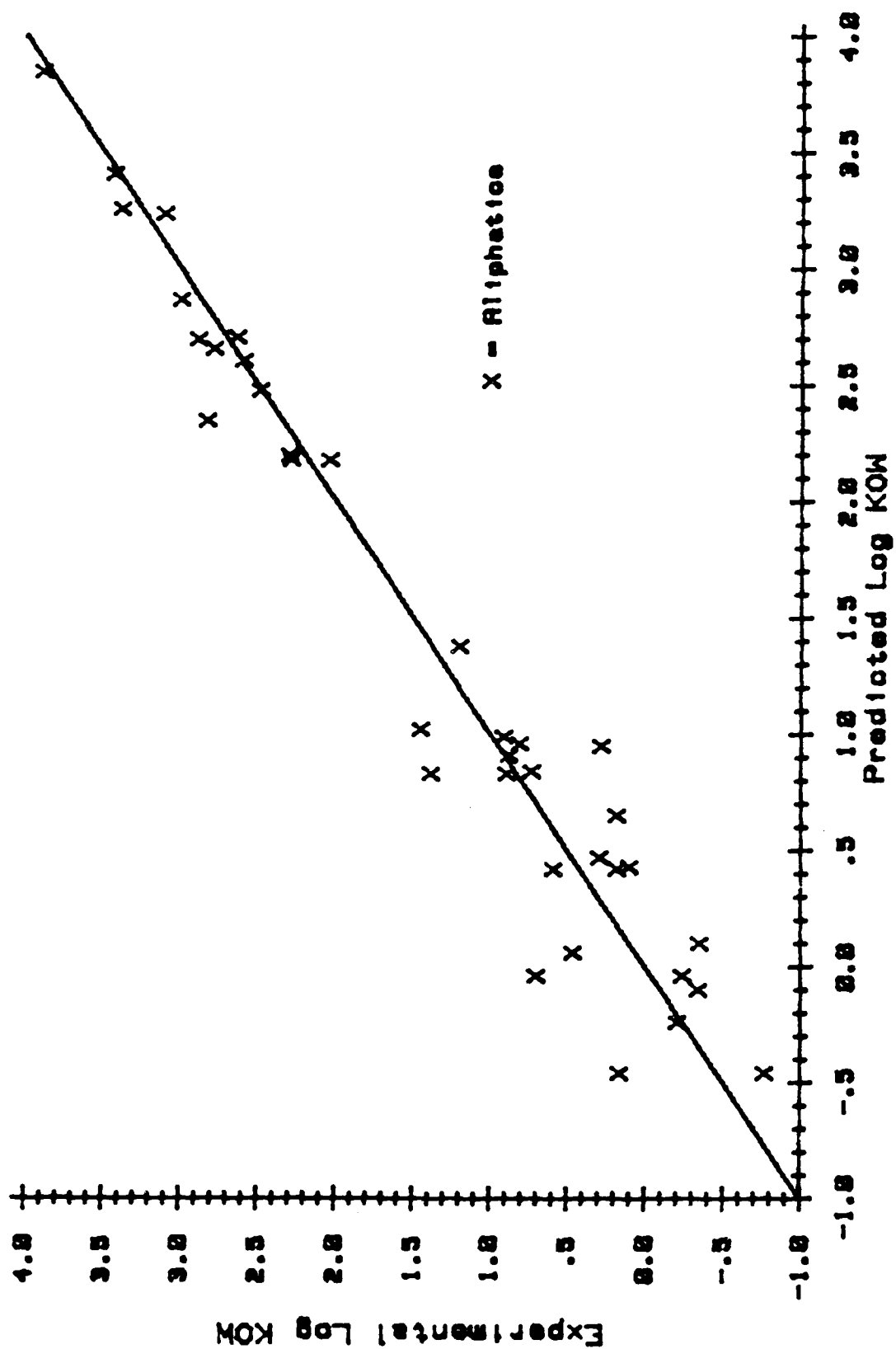


Figure 1. Octanol/Water Partition Coefficient: Theoretical LSER (Aliphatics)

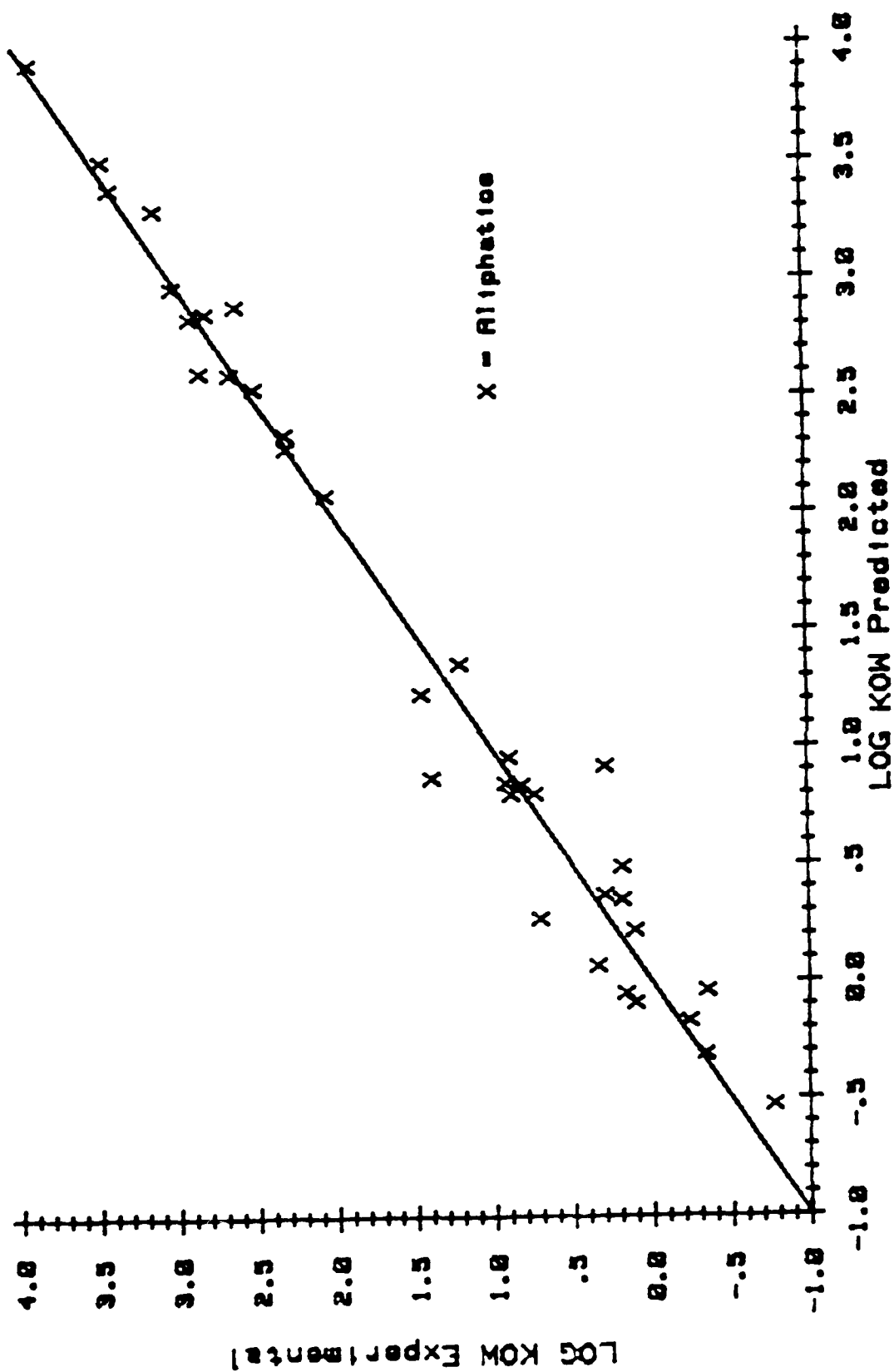


Figure 2. Octanol/Water Partition Coefficient: LSER (Aliphatics)

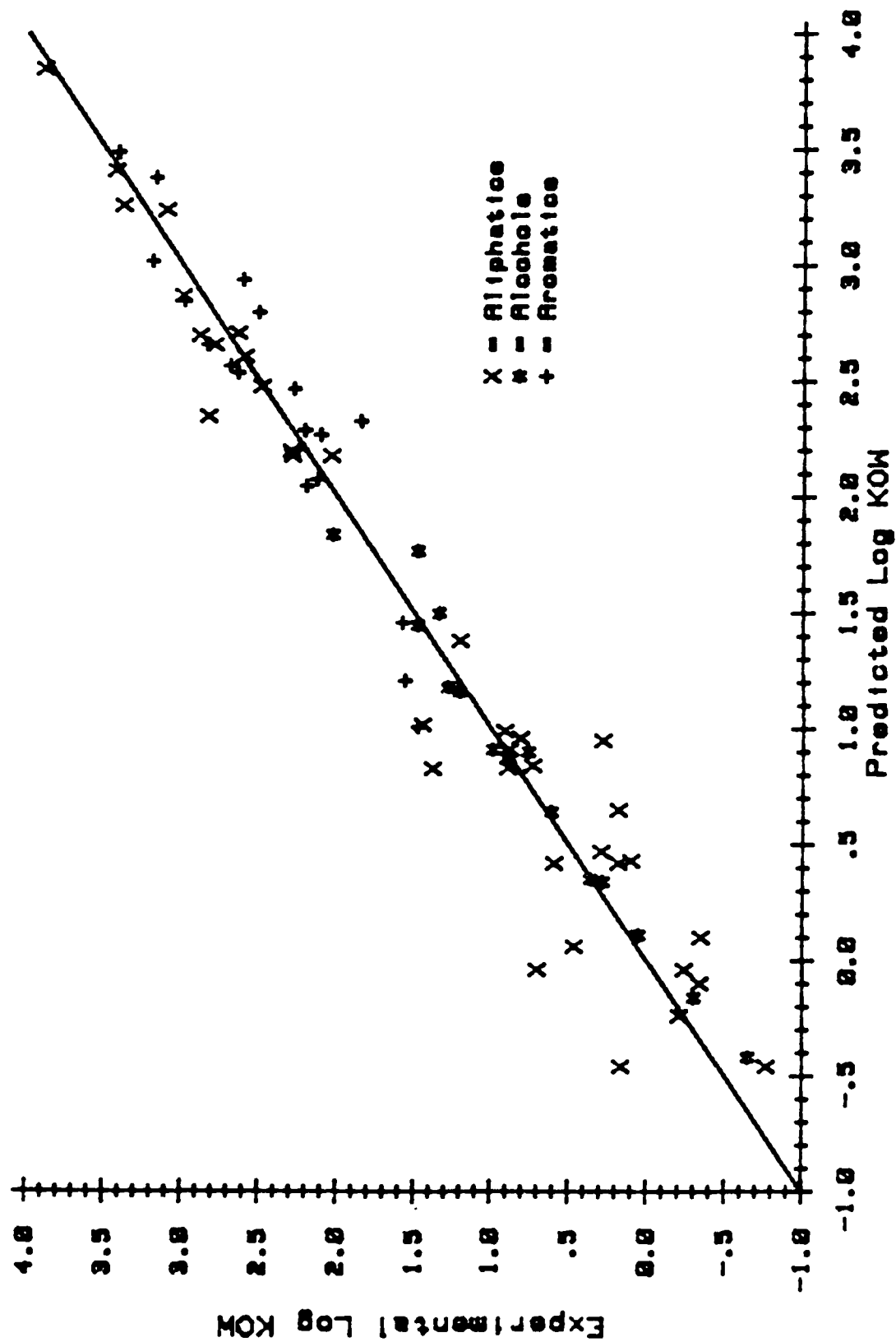


Figure 3. Octanol/Water Partition Coefficient: Theoretical LSER

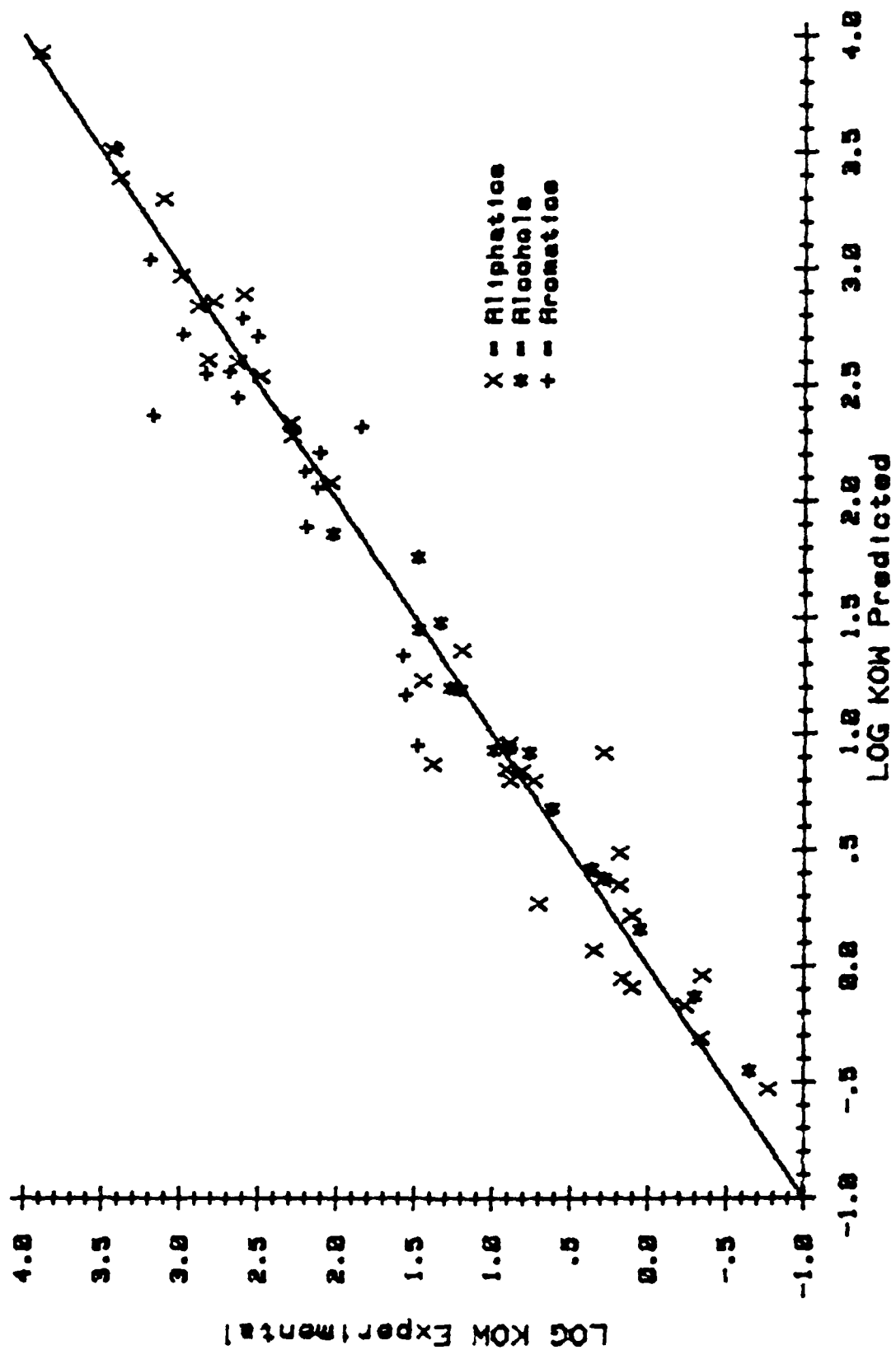


Figure 4. Octanol/Water Partition Coefficient: LSER

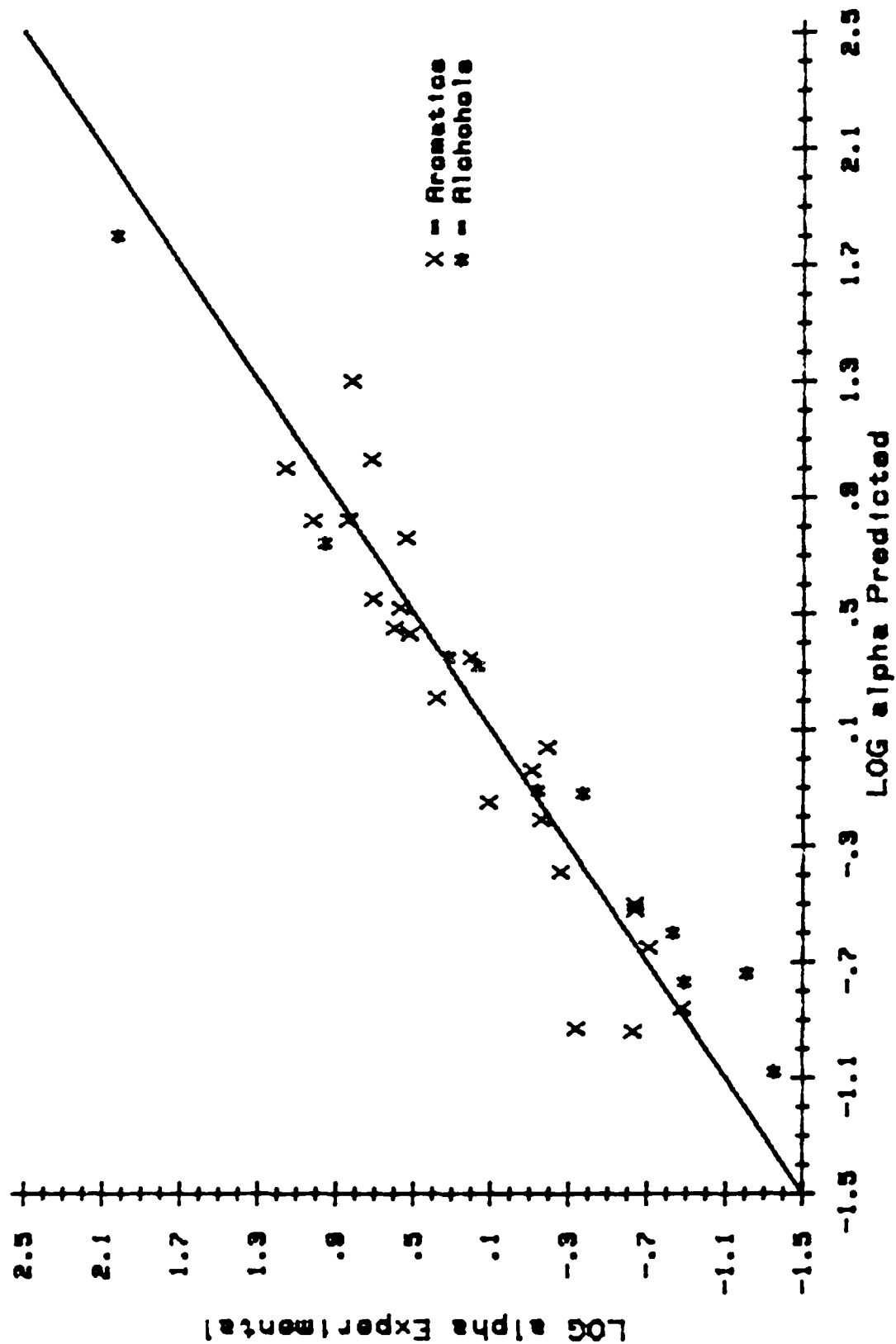


Figure 5. Charcoal Adsorbivity: Theoretical LSER

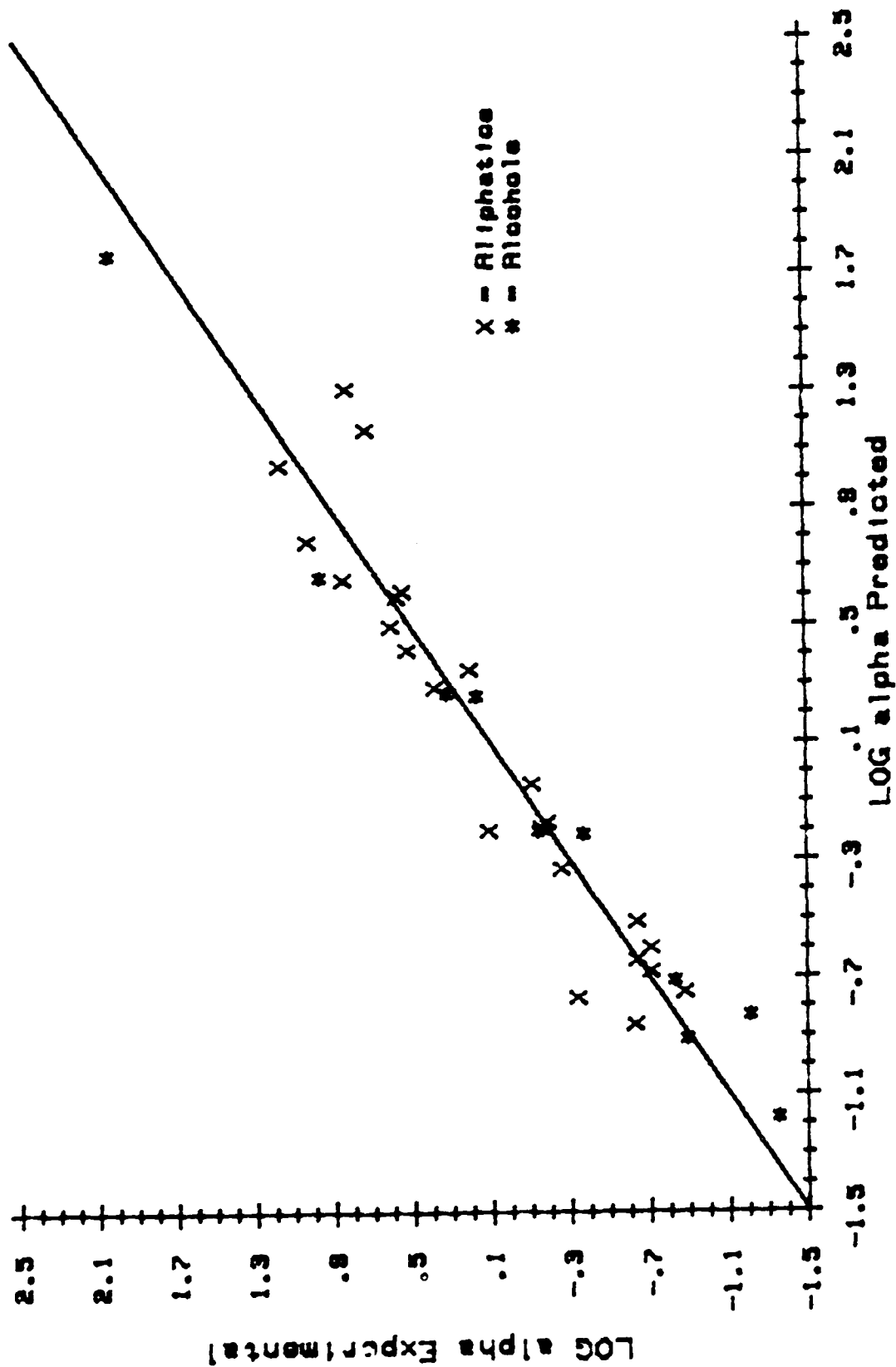


Figure 6. Charcoal Adsorbivity: LSER

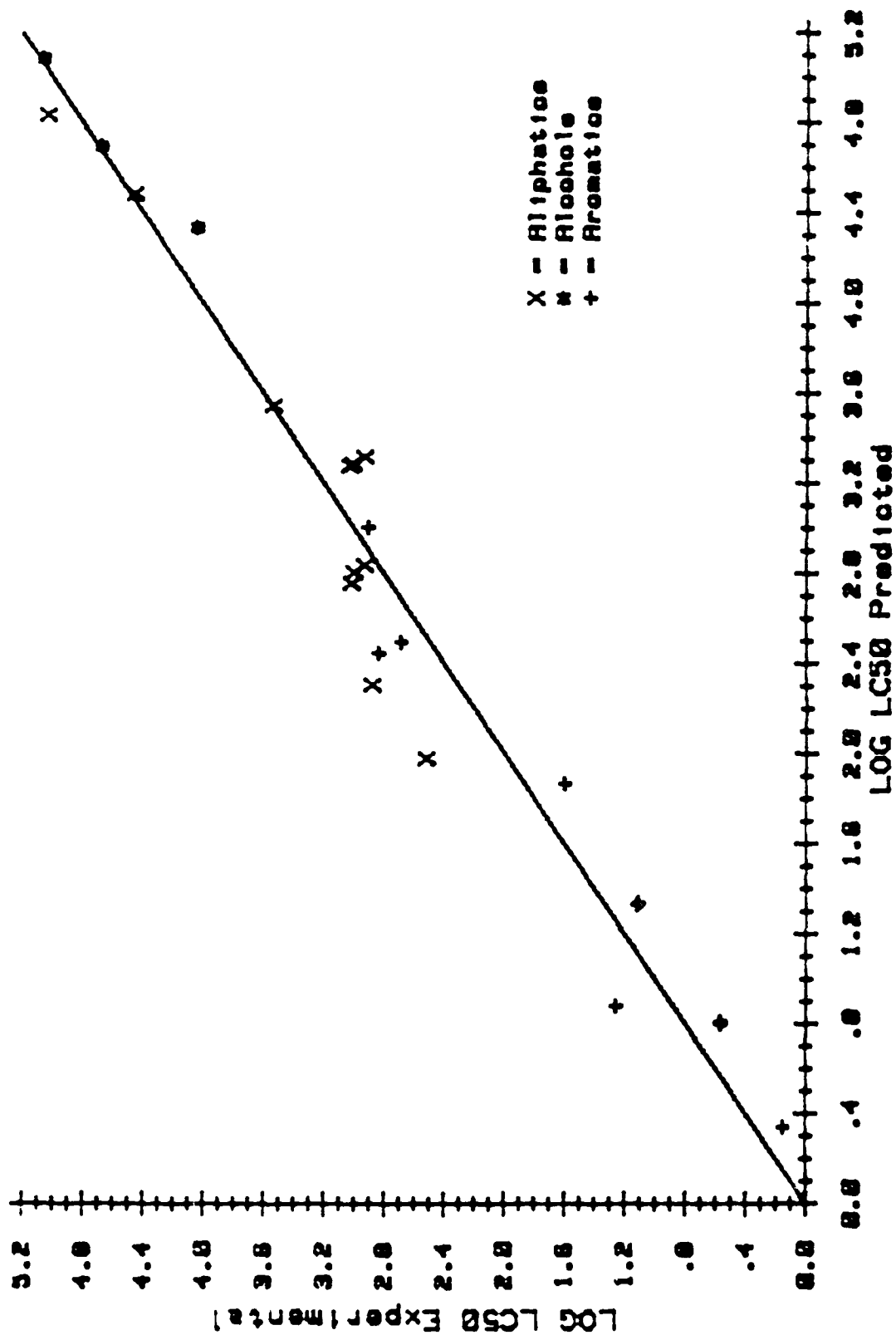


Figure 7. Konemann's Fish Toxicity: Theoretical I.S.E.R

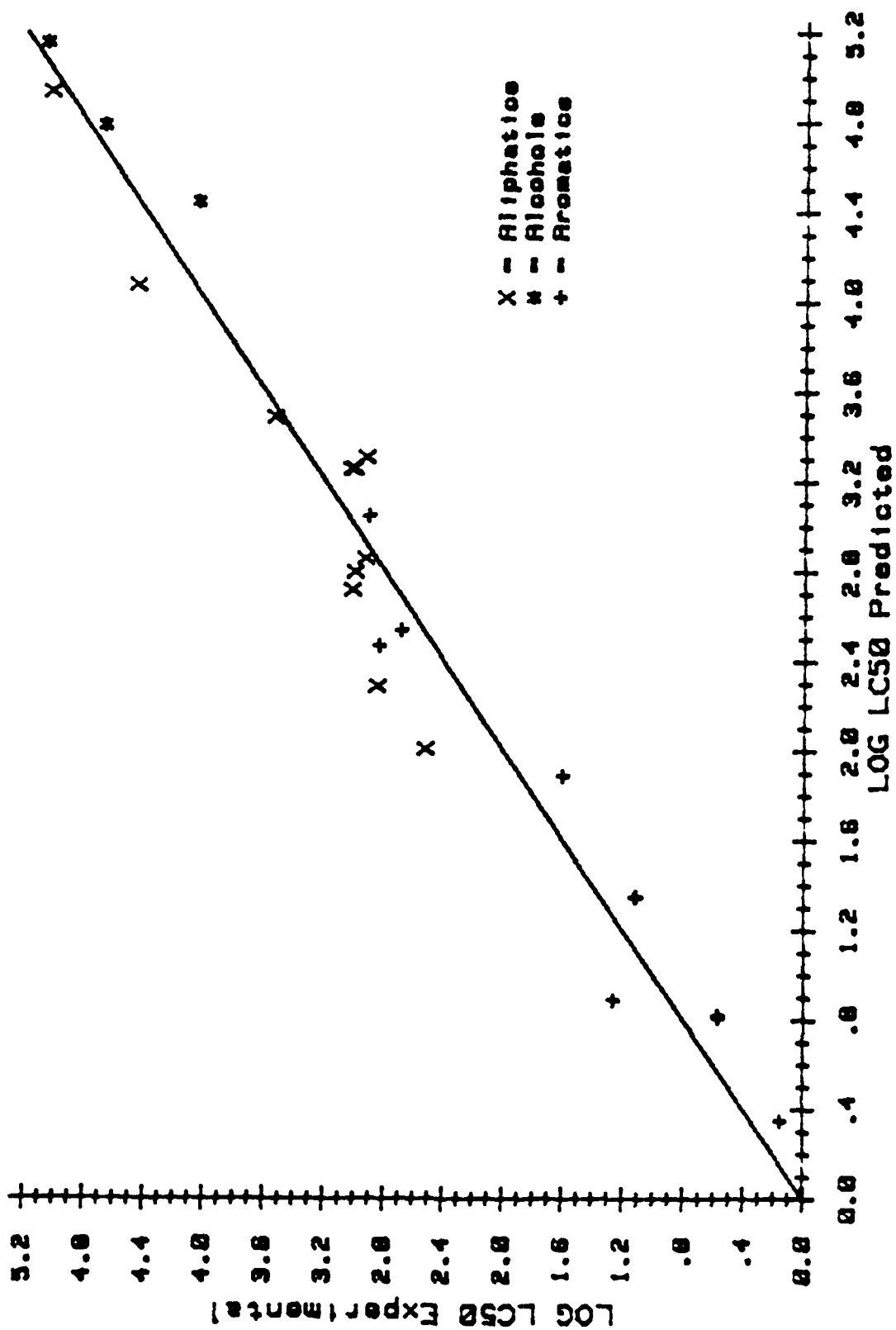


Figure 8. Konnemann's Fish Toxicity: LSER

TABLE 1. Compounds Used

ID Number	Compound Name	ID Number	Compound Name
mjk001	Hexane	mjk002	Cyclohexane
mjk005	Cyclopentane	mjk006	Butane
mjk007	1,1,2,2-Tetrachloroethylene	mjk008	Carbon Tetrachloride
mjk009	Tripropyl Amine	mjk011	1,1,1-Trichloroethane
mjk012	Propane	mjk013	1,1,2-Trichloroethylene
mjk014	Propyl Chloride	mjk015	Triethyl Amine
mjk016	2-Hexanone	mjk018	Ethyl Propionate
mjk019	2-Pentanone	mjk020	Diethyl Ether
mjk020	Diethyl Ether	mjk021	Butyraldehyde
mjk022	Cyclohexanone	mjk023	Ethyl Acetate
mjk024	Ethyl Dimethyl Amine	mjk025	Propanol
mjk026	Tetrahydrofuran	mjk028	Butanone
mjk029	Hexamethyl Phosphoramide	mjk03	Neopentane
mjk030	Methyl Acetate	mjk031	Nitroethane
mjk033	Propanonitrile	mjk034	Dimethyl Ether
mjk035	Methyl Acetate	mjk036	Acetonitrile
mjk037	Nitromethane	mjk038	Dimethyl Acetamide
mjk038	1,2-Dichloropropane	mjk039	Methanol
mjk04	Pentane	mjk040	Ethanol
mjk041	Propanol	mjk042	i-Propanol
mjk043	n-Butanol	mjk044	2-Methyl-1-Propanol
mjk045	2-Butanol	mjk046	t-Butanol
mjk047	n-Pentanol	mjk048	3-Pentanol
mjk049	2,2-Dimethyl-2-Butanol	mjk050	t-Pentanol
mjk051	3-Methyl-2-Butanol	mjk052	Hexanol
mjk053	3,3-Dimethyl-2-Butanol	mjk054	Benzene
mjk055	Ethyl Benzoate	mjk056	Acetophenone
mjk057	Dimethyl Aniline	mjk058	Benzaldehyde
mjk059	Toluene	mjk060	Methoxy Benzene
mjk061	Ethoxy Benzene	mjk062	Propyl Benzene
mjk063	1-Chlorobutane	mjk063	Chlorobenzene
mjk067	Mesitylene	mjk068	m-Xylene
mjk069	o-Methoxy Toluene	mjk070	N,N-DimethylAmino Toluene
mjk072	Phenyl Propanone	mjk085	Acetone

Table 1. (Continued)

ID Number	Compound Name	ID Number	Compound Name
mjk086	4-Methyl-2-Pentanone	mjk087	5-Methyl-2-Hexanone
mjk088	Propyl Acetate	mjk089	Butyl Acetate
mjk090	Amyl Acetate	mjk091	i-Propyl Acetate
mjk092	i-Butyl Acetate	mjk093	Valeraldehyde
mjk094	Acrolein	mjk095	Vinyl Acetate
mjk096	Di-n-Propyl Ether	mjk097	Di-i-Propyl Ether
mjk099	1,3-Dichloropropane	mjk010	Butyl Chloride
mjk100	2-Ethyl-1-Butanol	mjk101	2-Ethyl-1-Hexanol
mjk102	2-Propen-1-ol	mjk103	Cyclohexanol
mjk104	o-DichloroBenzene	mjk105	Dichloromethane
mjk106	Chloroform	mjk107	o-Xylene
mjk108	1,1-Dichloroethane	mjk109	1,1,2-Trichloroethane
mjk110	1,1,2,2-Tetrachloroethane	mjk111	1,2-Dichloroethane
mjk114	1,2,3-Trichlorobenzene	mjk115	1,2,4-Trichlorobenzene
mjk116	1,2,3,4-Tetrachlorobenzene	mjk117	1,2,3,5-Tetrachlorobenzene
mjk118	1,2,4,5-Tetrachlorobenzene	mjk119	Pentachlorobenzene
mjk120	2,5-Dichloro-m-xylene	mjk032	Trimethyl Amine

TABLE 2. Polarizability Index

ID Number	Compound Name	Molecular Volume	Polarizability Index
mjk040	Ethanol	54.2	.0927
mjk39	Methanol	36.5	.0859
mjk34	Dimethyl Ether	55.1	.0940
mjk36	Acetonitrile	45.1	.0941
mjk12	Propane	65.5	.0953
mjk042	i-Propanol	72.1	.0955
mjk41	Propanol	71.3	.0969
mjk085	Acetone	64.2	.0975
mjk33	Propanonitrile	63.1	.0975
mjk45	2-Butanol	89.7	.0976
mjk046	t-Butanol	89.1	.0978
mjk35	Methyl Acetate	63.9	.0979
mjk025	Propanol	64.3	.0979
mjk043	n-Butanol	89.8	.0980
mjk49	2,2-Dimethyl-2-Butanol	108.2	.0981
mjk044	2-Methyl-1-Propanol	89.4	.0982
mjk006	Butane	82.4	.0986
mjk051	3-Methyl-2-Butanol	107.2	.0992
mjk053	3,3-Dimethyl-2-Butanol	125.9	.0992
mjk020	Diethyl Ether	90.5	.0995
mjk50	t-Pentanol	106.5	.0996
mjk048	3-Pentanol	106.8	.0996
mjk047	n-Pentanol	106.8	.0995
mjk04	Pentane	100.4	.0996
mjk03	Neopentane	99.6	.0997
mjk01	Hexane	119.0	.1000
mjk019	2-Pentanone	100.1	.1001
mjk021	Butyraldehyde	81.6	.1002
mjk030	Methyl Acetate	70.8	.1005
mjk097	Di-i-Propyl Ether	126.2	.1006
mjk100	2-Ethyl-1-Butanol	124.1	.1008
mjk028	Butanone	81.0	.1009
mjk14	Propyl Chloride	80.9	.1010
mjk24	Ethyl Dimethyl Amine	96.2	.1010

Table 2. (Continued)

ID Number	Compound Name	Molecular Volume	Polarizability Index
mjk101	2-Ethyl-1-Hexanol	161.2	.1011
mjk087	5-Methyl-2-Hexanone	135.3	.1013
mjk086	4-Methyl-2-Pentanone	117.0	.1015
mjk023	Ethyl Acetate	88.9	.1018
mjk102	2-Propen-1-ol	64.2	.1018
mjk092	i-Butyl Acetate	125.1	.1020
mjk015	Triethyl Amine	131.5	.1020
mjk093	Valeraldehyde	98.8	.1020
mjk016	2-Hexanone	117.1	.1021
mjk18	Ethyl Propionate	107.3	.1022
mjk096	Di-n-Propyl Ether	125.2	.1023
mjk091	i-Propyl Acetate	106.5	.1024
mjk05	Cyclopentane	89.2	.1025
mjk10	Butyl Chloride	98.3	.1025
mjk26	Tetrahydrofuran	78.6	.1025
mjk088	Propyl Acetate	106.6	.1029
mjk105	Dichloromethane	60.5	.1035
mjk090	Amyl Acetate	142.2	.1036
mjk094	Acrolein	57.8	.1037
mjk089	Butyl Acetate	124.0	.1038
mjk052	Hexanol	121.1	.1039
mjk111	1,2-Dichloroethane	78.1	.1043
mjk02	Cyclohexane	106.7	.1045
mjk103	Cyclohexanol	113.1	.1049
mjk099	1,3-Dichloropropane	96.3	.1051
mjk09	Tripropyl Amine	181.6	.1052
mjk038	Dimethyl Acetamide	93.4	.1059
mjk038	1,2-Dichloropropane	95.3	.1061
mjk108	1,1-Dichloroethane	78.1	.1061
mjk22	Cyclohexanone	105.6	.1064
mjk32	Trimethyl Amine	78.0	.1066
mjk106	Chloroform	76.3	.1100
mjk37	Nitromethane	47.0	.1101
mjk095	Vinyl Acetate	81.7	.1104

Table 2. (Continued)

ID Number	Compound Name	Molecular Volume	Polarizability Index
mjk109	1,1,2-Trichloroethane	92.7	.1104
mjk31	Nitroethane	64.5	.1106
mjk11	1,1,1-Trichloroethane	94.1	.1109
mjk110	1,1,2,2-Tetrachloroethane	108.8	.1120
mjk29	Hexamethyl Phosphoramide	181.4	.1127
mjk008	Carbon Tetrachloride	91.6	.1159
mjk13	1,1,2-Trichloroethylene	86.2	.1162
mjk72	Phenyl Propanone	137.	.1186
mjk107	o-Xylene	119.9	.1199
mjk007	1,1,2,2-Tetrachloroethylene	101.3	.1204
mjk54	Benzene	84.6	.1204
mjk55	Ethyl Benzoate	143.1	.1204
mjk56	Acetophenone	119.1	.1204
mjk62	Propyl Benzene	144.3	.1208
mjk59	Toluene	101.8	.1209
mjk67	Mesitylene	136.5	.1210
mjk068	m-Xylene	118.9	.1212
mjk61	Ethoxy Benzene	126.4	.1224
mjk69	o-Methoxy Toluene	134.7	.1224
mjk63	Chloro Benzene	99.8	.1237
mjk60	Methoxy Benzene	109.	.1237
mjk58	Benzaldehyde	100.8	.1249
mjk57	Dimethyl Aniline	131.4	.1252
mjk70	N,N-DimethylAminoToluene	149.1	.1257
mjk104	o-DichloroBenzene	115.1	.1259
mjk120	2,5-Dichloro-m-xylene	149.4	.1259
mjk65	Cyano Benzene	99.7	.1276
mjk64	Bromo Benzene	105.8	.1280
mjk114	1,2,3-Trichlorobenzene	130.1	.1283
mjk115	1,2,4-Trichlorobenzene	130.2	.1290
mjk66	Nitro Benzene	101.7	.1307
mjk116	1,2,3,4-Tetrachlorobenzene	144.8	.1310
mjk117	1,2,3,5-Tetrachlorobenzene	145.1	.1311
mjk118	1,2,4,5-Tetrachlorobenzene	145.2	.1315
mjk119	Pentachlorobenzene	160.	.1331

TABLE 3. Theoretical LSER for Octanol/Water Partition Coefficient:
Aliphatics Only

ID Number	V _{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk01	119.00	0.1000	0.00	3.90	3.93	-0.03
mjk02	106.70	0.1045	0.00	3.44	3.45	-0.01
mjk03	99.60	0.0997	0.00	3.11	3.30	-0.19
mjk04	100.40	0.0997	0.00	3.39	3.33	0.06
mjk05	89.20	0.1025	0.00	3.00	2.91	0.09
mjk06	82.40	0.0986	0.00	2.89	2.76	0.13
mjk07	101.30	0.1204	0.10	2.60	2.54	0.06
mjk08	91.60	0.1159	0.10	2.83	2.30	0.53
mjk09	181.60	0.1052	0.69	2.79	2.74	0.05
mjk10	98.30	0.1025	0.10	2.64	2.75	-0.11
mjk11	94.10	0.1109	0.10	2.49	2.47	0.02
mjk12	65.50	0.0953	0.00	2.30	2.26	0.04
mjk13	86.20	0.1162	0.10	2.29	2.12	0.17
mjk14	80.90	0.1010	0.10	2.04	2.21	-0.17
mjk15	131.50	0.1020	0.71	1.45	1.06	0.39
mjk16	117.10	0.1021	0.65	1.38	0.86	0.52
mjk18	107.30	0.1022	0.46	1.20	1.41	-0.21
mjk19	100.10	0.1001	0.50	0.91	1.03	-0.12
mjk20	90.50	0.0995	0.47	0.89	0.86	0.03
mjk21	80.40	0.1002	0.38	0.88	0.93	-0.05
mjk22	105.60	0.1064	0.53	0.81	0.96	-0.15
mjk23	88.90	0.1018	0.45	0.73	0.86	-0.13
mjk24	96.20	0.1010	0.70	0.70	-0.03	0.73
mjk25	64.30	0.0979	0.38	0.59	0.44	0.15
mjk26	78.60	0.1025	0.55	0.34	0.05	0.29
mjk28	81.00	0.1009	0.48	0.29	0.48	-0.19
mjk29	181.40	0.1127	1.05	0.28	0.96	-0.68
mjk30	70.80	0.1005	0.42	0.18	0.42	-0.24
mjk32	78.00	0.1066	0.65	0.16	-0.50	0.66
mjk33	63.10	0.0975	0.37	0.10	0.45	-0.35
mjk34	55.10	0.0940	0.47	0.10	-0.21	0.31
mjk35	63.90	0.0979	0.48	-0.24	-0.03	-0.21
mjk36	45.10	0.0941	0.37	-0.34	-0.08	-0.26
mjk37	47.00	0.1101	0.30	-0.35	0.02	-0.37
mjk38	93.40	0.1059	0.76	-0.77	-0.48	-0.29

TABLE 4. LSER for Octanol/Water Partition Coefficient:
Aliphatics Only

ID Number	V_{mc}	π^*	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk01	119.00	-0.0800	0.00	3.90	3.88	0.02
mjk02	106.70	0.0000	0.00	3.44	3.46	-0.02
mjk03	99.60	0.0000	0.00	3.11	3.28	-0.17
mjk04	100.40	-0.0800	0.00	3.39	3.40	-0.01
mjk05	89.20	0.0000	0.00	3.00	3.01	-0.01
mjk06	82.40	-0.0800	0.00	2.89	2.94	-0.05
mjk07	101.30	0.0800	0.10	2.60	2.88	-0.28
mjk08	91.60	0.0800	0.10	2.83	2.63	0.20
mjk09	181.60	0.1400	0.69	2.79	2.81	-0.02
mjk10	98.30	0.3900	0.10	2.64	2.42	0.22
mjk11	94.10	0.2900	0.10	2.49	2.44	0.05
mjk12	65.50	-0.0800	0.00	2.30	2.50	-0.20
mjk13	86.20	0.3300	0.10	2.29	2.18	0.11
mjk14	80.90	0.3900	0.10	2.04	1.98	0.06
mjk15	131.50	0.2400	0.71	1.45	1.33	0.12
mjk16	117.10	0.5000	0.65	1.38	0.85	0.53
mjk18	107.30	0.4700	0.46	1.20	1.30	-0.10
mjk19	100.10	0.6700	0.50	0.91	0.73	0.18
mjk20	90.50	0.2700	0.47	0.89	1.08	-0.19
mjk21	80.40	0.6000	0.38	0.88	0.73	0.15
mjk22	105.60	0.7600	0.53	0.81	0.66	0.15
mjk23	88.90	0.5500	0.45	0.73	0.76	-0.03
mjk24	96.20	0.1600	0.70	0.70	0.55	0.15
mjk25	64.30	0.6000	0.38	0.59	0.32	0.27
mjk26	78.60	0.5800	0.55	0.34	0.11	0.23
mjk28	81.00	0.6700	0.48	0.29	0.31	-0.02
mjk29	181.40	0.8700	1.05	0.28	0.66	-0.38
mjk30	70.80	0.6000	0.42	0.18	0.34	-0.16
mjk32	78.00	0.1400	0.65	0.16	0.28	-0.12
mjk33	63.10	0.7500	0.37	0.10	0.14	-0.04
mjk34	55.10	0.2700	0.47	0.10	0.17	-0.07
mjk35	63.90	0.7100	0.48	-0.24	-0.18	-0.06
mjk36	45.10	0.7500	0.37	-0.34	-0.32	-0.02
mjk37	47.00	0.8500	0.30	-0.35	-0.15	-0.20
mjk38	93.40	0.8800	0.76	-0.77	-0.60	-0.17

TABLE 5. Theoretical LSER for Octanol/Water Partition Coefficient:
Aliphatics and Alcohols

ID Number	V_{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk01	119.00	0.1000	0.00	3.90	3.91	-0.01
mjk02	106.70	0.1045	0.00	3.44	3.45	-0.01
mjk03	99.60	0.0997	0.00	3.11	3.28	-0.17
mjk04	100.40	0.0997	0.00	3.39	3.30	0.09
mjk05	89.20	0.1025	0.00	3.00	2.90	0.10
mjk06	82.40	0.0986	0.00	2.89	2.73	0.16
mjk07	101.30	0.1204	0.10	2.60	2.62	-0.02
mjk08	91.60	0.1159	0. 0.1162	0.12	0.29	2.08
mjk14	80.90	0.1010	0.12	0.04	2.10	-2.06
mjk15	131.50	0.1020	0.71	0.45	1.03	-0.58
mjk16	117.10	0.1021	0.65	0.38	0.83	-0.45
mjk18	107.30	0.1022	0.46	0.20	1.38	-1.18
mjk19	100.10	0.1001	0.50	0.91	0.99	-0.08
mjk20	90.50	0.0995	0.47	0.89	0.82	0.07
mjk21	80.40	0.1002	0.38	0.88	0.89	-0.01
mjk22	105.60	0.1064	0.53	0.81	0.96	-0.15
mjk23	88.90	0.1018	0.45	0.73	0.83	-0.10
mjk24	96.20	0.1010	0.70	0.70	-0.07	0.77
mjk25	64.30	0.0979	0.38	0.59	0.39	0.20
mjk26	78.60	0.1025	0.55	0.34	0.03	0.31
mjk28	81.00	0.1009	0.48	0.29	0.45	-0.16
mjk29	181.40	0.1127	0.05	0.28	5.57	-5.29
mjk30	70.80	0.1005	0.42	0.18	0.39	-0.21
mjk31	64.50	0.1106	0.30	0.18	0.61	-0.43
mjk32	78.00	0.1066	0.65	0.16	-0.50	0.66
mjk33	63.10	0.0975	0.37	0.10	0.41	-0.31
mjk34	55.10	0.0940	0.47	0.10	-0.27	0.37

Table 5. (Continued)

ID Number	V_{mc}	π_I	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk35	63.90	0.0979	0.48	0.24	-0.08	0.32
mjk36	45.10	0.0941	0.37	0.34	-0.14	0.48
mjk37	47.00	0.1101	0.30	0.35	0.04	0.31
mjk38	93.40	0.1059	0.76	0.77	-0.50	1.27
mjk39	36.50	0.0859	0.40	0.65	-0.46	1.11
mjk40	54.20	0.0927	0.45	0.30	-0.20	0.50
mjk41	71.30	0.0969	0.45	0.28	0.31	-0.03
mjk42	72.10	0.0955	0.51	0.05	0.08	-0.03
mjk43	89.80	0.0980	0.45	0.99	0.91	0.08
mjk44	89.40	0.0982	0.45	0.76	0.89	-0.13
mjk45	89.70	0.0976	0.51	0.61	0.63	-0.02
mjk46	89.10	0.0978	0.57	0.36	0.34	0.02
mjk47	107.40	0.0995	0.45	0.48	1.46	-0.98
mjk48	106.80	0.0996	0.51	0.21	1.17	-0.96
mjk49	108.20	0.0981	0.45	0.34	1.51	-1.17
mjk50	106.50	0.0996	0.57	0.89	0.89	0.00
mjk51	107.20	0.0992	0.51	0.28	1.19	-0.91
mjk52	121.10	0.1039	0.45	0.03	1.85	-1.82
mjk53	125.90	0.0992	0.51	0.48	1.80	-1.32

TABLE 6. LSER for Octanol/Water Partition Coefficient:
Aliphatics and Alcohols

ID Number	V _{mc}	π	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk01	119.00	-0.0800	0.00	3.90	3.91	-0.01
mjk02	106.70	0.0000	0.00	3.44	3.49	-0.05
mjk03	99.60	0.0000	0.00	3.11	3.29	-0.18
mjk04	100.40	-0.0800	0.00	3.39	3.40	-0.01
mjk05	89.20	0.0000	0.00	3.00	3.00	0.00
mjk06	82.40	-0.0800	0.00	2.89	2.90	-0.01
mjk07	101.30	0.0800	0.10	2.60	2.88	-0.28
mjk08	91.60	0.0800	0.10	2.83	2.61	0.22
mjk09	181.60	0.1400	0.69	2.79	2.85	-0.06
mjk10	98.30	0.3900	0.10	2.64	2.46	0.18
mjk11	94.10	0.2900	0.10	2.49	2.45	0.04
mjk12	65.50	-0.0800	0.00	2.30	2.43	-0.13
mjk13	86.20	0.3300	0.12	0.29	2.12	-1.83
mjk14	80.90	0.3900	0.12	0.04	1.91	-1.87
mjk15	131.50	0.2400	0.71	0.45	1.28	-0.83
mjk16	117.10	0.5000	0.65	0.38	0.82	-0.44
mjk18	107.30	0.4700	0.46	0.20	1.29	-1.09
mjk19	100.10	0.6700	0.50	0.91	0.73	0.18
mjk20	90.50	0.2700	0.47	0.89	1.01	-0.12
mjk21	80.40	0.6000	0.38	0.88	0.70	0.18
mjk22	105.60	0.7600	0.53	0.81	0.67	0.14
mjk23	88.90	0.5500	0.45	0.73	0.73	0.00
mjk24	96.20	0.1600	0.70	0.70	0.43	0.27
mjk25	64.30	0.6000	0.38	0.59	0.26	0.33
mjk26	78.60	0.5800	0.55	0.34	0.05	0.29
mjk28	81.00	0.6700	0.48	0.29	0.28	0.01
mjk29	181.40	0.8710	0.05	0.28	4.43	-4.15
mjk30	70.80	0.6000	0.42	0.18	0.29	-0.11
mjk31	64.50	0.8300	0.30	0.18	0.31	-0.13
mjk32	78.00	0.1400	0.65	0.16	0.13	0.03
mjk33	63.10	0.7500	0.37	0.10	0.10	0.00
mjk34	55.10	0.2700	0.47	0.10	0.03	0.07

Table 6. (Continued)

ID Number	V_{inc}	π_I	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk35	63.90	0.7100	0.48	0.24	-0.24	0.48
mjk36	45.10	0.7500	0.37	0.34	-0.40	0.74
mjk37	47.00	0.8500	0.30	0.35	-0.19	0.54
mjk38	93.40	0.8800	0.76	0.77	-0.64	1.41
mjk39	36.50	0.4000	0.40	0.65	-0.37	1.02
mjk40	54.20	0.4000	0.45	0.30	-0.06	0.36
mjk41	71.30	0.4000	0.45	0.28	0.41	-0.13
mjk42	72.10	0.4000	0.51	0.05	0.21	-0.16
mjk43	89.80	0.4000	0.45	0.99	0.92	0.07
mjk44	89.40	0.4000	0.45	0.76	0.91	-0.15
mjk45	89.70	0.4000	0.51	0.61	0.70	-0.09
mjk46	89.10	0.4000	0.57	0.36	0.46	-0.10
mjk47	107.40	0.4000	0.45	0.48	1.40	-0.92
mjk48	106.80	0.4000	0.51	0.21	1.17	-0.96
mjk49	108.20	0.4000	0.45	0.34	1.43	-1.09
mjk50	106.50	0.4000	0.57	0.89	0.94	-0.05
mjk51	107.20	0.4000	0.51	0.28	1.18	-0.90
mjk52	121.10	0.4000	0.45	0.03	1.78	-1.75
mjk53	125.90	0.4000	0.51	0.48	1.69	-1.21

TABLE 7. Theoretical LSER for Octanol/Water Partition Coefficient:
Aliphatics, Alcohols, and Aromatics

ID Number	V_{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk01	119.00	0.1000	0.00	3.90	3.85	0.05
mjk02	106.70	0.1045	0.00	3.44	3.41	0.03
mjk03	99.60	0.0997	0.00	3.11	3.24	-0.13
mjk04	100.40	0.0997	0.00	3.39	3.26	0.13
mjk05	89.20	0.1025	0.00	3.00	2.87	0.13
mjk06	82.40	0.0986	0.00	2.89	2.70	0.19
mjk07	101.30	0.1204	0.12	0.60	2.52	-1.92
mjk08	91.60	0.1159	0.12	0.83	2.26	-1.43
mjk09	181.60	0.1052	0.69	0.79	2.66	-1.87
mjk10	98.30	0.1025	0.12	0.64	2.62	-1.98
mjk11	94.10	0.1109	0.12	0.49	2.39	-1.90
mjk12	65.50	0.0953	0.00	2.30	2.20	0.10
mjk13	86.20	0.1162	0.12	0.29	2.09	-1.80
mjk14	80.90	0.1010	0.12	0.04	2.09	-2.05
mjk15	131.50	0.1020	0.71	0.45	1.02	-0.57
mjk16	117.10	0.1021	0.65	0.38	0.83	-0.45
mjk18	107.30	0.1022	0.46	0.20	1.37	-1.17
mjk19	100.10	0.1001	0.50	0.91	0.99	-0.08
mjk20	90.50	0.0995	0.47	0.89	0.83	0.06
mjk21	80.40	0.1002	0.38	0.88	0.91	-0.03
mjk22	105.60	0.1064	0.53	0.81	0.96	-0.15
mjk23	88.90	0.1018	0.45	0.73	0.84	-0.11
mjk24	96.20	0.1010	0.70	0.70	-0.05	0.75
mjk25	74.30	0.0979	0.38	0.59	0.42	0.17
mjk26	78.60	0.1025	0.55	0.34	0.06	0.28
mjk28	81.00	0.1009	0.48	0.29	0.47	-0.18
mjk29	181.40	0.1127	0.05	0.28	5.46	-5.18
mjk30	70.80	0.1005	0.42	0.18	0.42	-0.24
mjk31	64.50	0.1106	0.30	0.18	0.65	-0.47
mjk32	78.00	0.1066	0.65	0.16	-0.46	0.62
mjk33	63.10	0.0975	0.37	0.10	0.43	-0.33
mjk34	55.10	0.0940	0.47	0.10	-0.24	0.34
mjk35	63.90	0.0979	0.48	0.24	-0.04	0.28
mjk36	45.10	0.0941	0.37	0.34	-0.10	0.44
mjk37	47.00	0.1101	0.30	0.35	0.10	0.25

Table 7. (Continued)

ID Number	V _{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk38	93.40	0.1059	0.76	0.77	-0.46	1.23
mjk39	36.50	0.0859	0.40	0.65	-0.42	1.07
mjk40	54.20	0.0927	0.45	0.30	-0.16	0.46
mjk41	71.30	0.0969	0.45	0.28	0.34	-0.06
mjk42	72.10	0.0955	0.51	0.05	0.11	-0.06
mjk43	89.80	0.0980	0.45	0.99	0.91	0.08
mjk44	89.40	0.0982	0.45	0.76	0.90	-0.14
mjk45	89.70	0.0976	0.51	0.61	0.64	-0.03
mjk46	89.10	0.0978	0.57	0.36	0.35	0.01
mjk47	107.40	0.0995	0.45	0.48	1.45	-0.97
mjk48	106.80	0.0996	0.51	0.21	1.16	-0.95
mjk49	108.20	0.0981	0.45	0.34	1.49	-1.15
mjk50	106.50	0.0996	0.57	0.89	0.88	0.01
mjk51	107.20	0.0992	0.51	0.28	1.18	-0.90
mjk52	121.10	0.1039	0.45	0.03	1.83	-1.80
mjk53	125.90	0.0992	0.51	0.48	1.77	-1.29
mjk54	84.60	0.1204	0.10	0.13	2.07	-1.94
mjk55	143.10	0.1204	0.41	0.64	2.53	-1.89
mjk56	119.10	0.1204	0.48	0.58	1.45	-0.87
mjk57	131.40	0.1252	0.33	0.28	2.46	-2.18
mjk58	100.80	0.1249	0.44	0.48	1.00	-0.52
mjk59	101.80	0.1209	0.11	0.69	2.56	-1.87
mjk60	109.00	0.1237	0.22	0.11	2.27	-2.16
mjk61	126.40	0.1224	0.23	0.51	2.79	-2.28
mjk62	144.30	0.1208	0.23	0.18	3.37	-3.19
mjk63	99.80	0.1237	0.07	0.84	2.65	-1.81
mjk64	105.80	0.1280	0.06	0.99	2.84	-1.85
mjk65	99.70	0.1276	0.38	0.56	1.21	-0.65
mjk66	101.70	0.1307	0.14	0.85	2.32	-1.47
mjk67	136.50	0.1210	0.15	0.42	3.48	-3.06
mjk35	63.90	0.7100	0.48	0.24	-0.17	0.41
mjk68	118.90	0.1212	0.13	0.20	3.01	-2.81
mjk69	134.70	0.1224	0.40	0.21	2.28	-2.07
mjk70	149.10	0.1257	0.35	0.61	2.93	-2.32
mjk72	137.00	0.1186	0.48	0.20	2.04	-1.84

TABLE 8. LSER for Octanol/Water Partition Coefficient:
Aliphatics, Alcohols, and Aromatics

ID Number	V _{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk01	119.00	-0.0800	0.00	3.90	3.93	-0.03
mjk02	106.70	0.0000	0.00	3.44	3.51	-0.07
mjk03	99.60	0.0000	0.00	3.11	3.30	-0.19
mjk04	100.40	-0.0800	0.00	3.39	3.38	0.01
mjk05	89.20	0.0000	0.00	3.00	2.99	0.01
mjk06	82.40	-0.0800	0.00	2.89	2.84	0.05
mjk07	101.30	0.0800	0.12	0.60	2.81	-2.21
mjk08	91.60	0.0800	0.12	0.83	2.53	-1.70
mjk09	181.60	0.1400	0.69	0.79	2.85	-2.06
mjk10	98.30	0.3900	0.12	0.64	2.52	-1.88
mjk11	94.10	0.2900	0.12	0.49	2.46	-1.97
mjk12	65.50	-0.0800	0.00	2.30	2.34	-0.04
mjk13	86.20	0.3300	0.12	0.29	2.20	-1.91
mjk14	80.90	0.3900	0.12	0.04	2.00	-1.96
mjk15	131.50	0.2400	0.71	0.45	1.22	-0.77
mjk16	117.10	0.5000	0.65	0.38	0.86	-0.48
mjk18	107.30	0.4700	0.46	0.20	1.36	-1.16
mjk19	100.10	0.6700	0.50	0.91	0.85	0.06
mjk20	90.50	0.2700	0.47	0.89	0.96	-0.07
mjk21	80.40	0.6000	0.38	0.88	0.80	0.08
mjk22	105.60	0.7600	0.53	0.81	0.84	-0.03
mjk23	88.90	0.5500	0.45	0.73	0.80	-0.07
mjk24	96.20	0.1600	0.70	0.70	0.27	0.43
mjk25	64.30	0.6000	0.38	0.59	0.32	0.27
mjk26	78.60	0.5800	0.55	0.34	0.07	0.27
mjk28	81.00	0.6700	0.48	0.29	0.37	-0.08
mjk29	181.40	0.8710	0.05	0.28	4.95	-4.67
mjk30	70.80	0.6000	0.42	0.18	0.35	-0.17
mjk31	64.50	0.8300	0.30	0.18	0.50	-0.32
mjk32	78.00	0.1400	0.65	0.16	-0.05	0.21
mjk33	63.10	0.7500	0.37	0.10	0.22	-0.12
mjk34	55.10	0.2700	0.47	0.10	-0.10	0.20
mjk35	63.90	0.7100	0.48	0.24	-0.17	0.41
mjk36	45.10	0.7500	0.37	0.34	-0.31	0.65
mjk37	47.00	0.8500	0.30	0.35	-0.04	0.39
mjk38	93.40	0.8800	0.76	0.77	-0.53	1.30

Table 8. (Continued)

ID Number	V_{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk39	36.50	0.4000	0.40	0.65	-0.45	1.10
mjk40	54.20	0.4000	0.45	0.30	-0.13	0.43
mjk41	71.30	0.4000	0.45	0.28	0.38	-0.10
mjk42	72.10	0.4000	0.51	0.05	0.16	-0.11
mjk43	89.80	0.4000	0.45	0.99	0.93	0.06
mjk44	89.40	0.4000	0.45	0.76	0.92	-0.16
mjk45	89.70	0.4000	0.51	0.61	0.68	-0.07
mjk46	89.10	0.4000	0.57	0.36	0.42	-0.06
mjk47	107.40	0.4000	0.45	0.48	1.45	-0.97
mjk48	106.80	0.4000	0.51	0.21	1.19	-0.98
mjk49	108.20	0.4000	0.45	0.34	1.47	-1.13
mjk50	106.50	0.4000	0.57	0.89	0.94	-0.05
mjk51	107.20	0.4000	0.51	0.28	1.20	-0.92
mjk52	121.10	0.4000	0.45	0.03	1.85	-1.82
mjk53	125.90	0.4000	0.51	0.48	1.76	-1.28
mjk54	84.60	0.5900	0.10	0.13	2.05	-1.92
mjk55	143.10	0.7400	0.41	0.64	2.44	-1.80
mjk56	119.10	0.9000	0.48	0.58	1.34	-0.76
mjk57	131.40	0.9000	0.33	0.28	2.31	-2.03
mjk58	100.80	0.9200	0.44	0.48	0.94	-0.46
mjk59	101.80	0.5400	0.11	0.69	2.55	-1.86
mjk60	109.00	0.7300	0.22	0.11	2.20	-2.09
mjk61	126.40	0.6900	0.23	0.51	2.70	-2.19
mjk62	144.30	0.6500	0.23	0.18	3.26	-3.08
mjk63	99.80	0.7100	0.07	0.84	2.54	-1.70
mjk64	105.80	0.7900	0.06	0.99	2.71	-1.72
mjk65	99.70	0.9000	0.38	0.56	1.17	-0.61
mjk66	101.70	0.7000	0.14	0.85	2.33	-1.48
mjk67	136.50	0.4100	0.15	0.42	3.51	-3.09
mjk35	63.90	0.7100	0.48	0.24	-0.17	0.41
mjk68	118.90	0.4700	0.13	0.20	3.02	-2.82
mjk69	134.70	0.9000	0.40	0.21	2.12	-1.91
mjk70	149.10	0.8500	0.35	0.61	2.78	-2.17
mjk72	137.00	0.8800	0.48	0.20	1.88	-1.68

TABLE 9. Theoretical LSER for Charcoal Adsorbitivity

ID Number	V _{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk085	64.20	0.0975	0.48	-0.88	-0.87	-0.01
mjk028	81.00	0.1009	0.68	-0.34	-0.93	0.59
mjk019	100.10	0.1001	0.50	-0.19	0.04	-0.23
mjk016	117.10	0.1021	0.50	0.64	0.50	0.14
mjk086	117.00	0.1015	0.48	0.71	0.55	0.16
mjk087	135.30	0.1013	0.48	0.72	1.03	-0.31
mjk030	70.80	0.1005	0.42	-0.64	-0.53	-0.11
mjk023	88.90	0.1018	0.42	-0.11	-0.04	-0.07
mjk088	106.60	0.1029	0.42	0.52	0.43	0.09
mjk089	124.00	0.1038	0.45	1.02	0.82	0.20
mjk090	142.20	0.1036	0.45	0.82	1.30	-0.48
mjk091	106.50	0.1024	0.45	0.20	0.35	-0.15
mjk092	125.10	0.1020	0.60	0.60	0.45	0.15
mjk025	64.30	0.0979	0.40	-0.71	-0.65	-0.06
mjk021	81.60	0.1002	0.41	0.16	-0.21	0.37
mjk093	98.80	0.1020	0.41	0.38	0.25	0.13
mjk094	57.80	0.1037	0.45	-0.63	-0.94	0.31
mjk095	81.70	0.1104	0.40	0.11	-0.16	0.27
mjk020	90.40	0.0100	0.47	-0.26	-0.40	0.14
mjk096	125.20	0.1023	0.46	0.84	0.82	0.02
mjk097	126.20	0.1006	0.49	0.54	0.76	-0.22
mjk098	78.30	0.1050	0.10	0.57	0.52	0.05
mjk099	96.30	0.1051	0.10	1.16	1.00	0.16
mjk040	54.20	0.0859	0.45	-1.35	-1.09	-0.26
mjk041	71.30	0.0969	0.45	-0.83	-0.60	-0.23
mjk043	89.80	0.0980	0.45	-0.14	-0.11	-0.03
mjk047	106.80	0.0996	0.45	0.32	0.35	-0.03
mjk052	121.10	0.1039	0.45	0.96	0.74	0.22
mjk042	72.00	0.0959	0.51	-1.21	-0.74	-0.47
mjk044	89.40	0.0982	0.45	-0.37	-0.12	-0.25
mjk101	161.20	0.1011	0.45	2.03	1.80	0.23
mjk102	64.20	0.1018	0.45	-0.89	-0.77	-0.12
mjk103	113.10	0.1049	0.53	0.17	0.32	-0.15

TABLE 10. LSER for Charcoal Adsorbtivity

ID Number	V_{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk085	64.20	0.7100	0.48	-0.88	-0.74	-0.14
mjk028	81.00	0.6800	0.68	-0.34	-0.76	0.42
mjk019	100.10	0.6700	0.50	-0.19	0.18	-0.37
mjk016	117.10	0.6700	0.50	0.64	0.65	-0.01
mjk086	117.00	0.6700	0.48	0.71	0.69	0.02
mjk087	135.30	0.6500	0.48	0.72	1.18	-0.46
mjk030	70.80	0.6000	0.42	-0.64	-0.50	-0.14
mjk023	88.90	0.5500	0.42	-0.11	-0.04	-0.07
mjk088	106.60	0.5200	0.42	0.52	0.43	0.09
mjk089	124.00	0.4600	0.45	1.02	0.80	0.22
mjk090	142.20	0.4800	0.45	0.82	1.32	-0.50
mjk091	106.50	0.5200	0.45	0.20	0.36	-0.16
mjk092	125.10	0.5000	0.60	0.60	0.51	0.09
mjk025	64.30	0.6500	0.40	-0.71	-0.60	-0.11
mjk021	81.60	0.6000	0.41	0.16	-0.18	0.34
mjk093	98.80	0.6000	0.41	0.38	0.30	0.08
mjk094	57.80	0.7000	0.45	-0.63	-0.85	0.22
mjk095	81.70	0.5500	0.40	0.11	-0.19	0.30
mjk020	90.40	0.2700	0.47	-0.26	-0.32	0.06
mjk096	125.20	0.2700	0.46	0.84	0.67	0.17
mjk097	126.20	0.2700	0.49	0.54	0.63	-0.09
mjk098	78.30	0.8100	0.10	0.57	0.60	-0.03
mjk099	96.30	0.7500	0.10	1.16	1.06	0.10
mjk040	54.20	0.4000	0.45	-1.35	-1.18	-0.17
mjk041	71.30	0.4000	0.45	-0.83	-0.70	-0.13
mjk043	89.80	0.4000	0.45	-0.14	-0.19	0.05
mjk047	106.80	0.4000	0.45	0.32	0.28	0.04
mjk052	121.10	0.4000	0.45	0.96	0.67	0.29
mjk042	72.00	0.4000	0.51	-1.21	-0.82	-0.39
mjk044	89.40	0.4000	0.45	-0.37	-0.20	-0.17
mjk101	161.20	0.4000	0.45	2.03	1.78	0.25
mjk102	64.20	0.4000	0.45	-0.89	-0.90	0.01
mjk103	113.10	0.4000	0.53	0.17	0.27	-0.10

TABLE 11. Theoretical LSER for Konnemann's Fish Toxicity

ID Number	V_{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk54	84.60	0.1204	0.10	2.91	3.05	-0.14
mjk59	101.80	0.1209	0.11	2.69	2.55	0.14
mjk63	99.80	0.1208	0.07	2.84	2.48	0.36
mjk104	115.10	0.1259	0.04	1.60	1.89	-0.29
mjk105	60.50	0.1035	0.00	3.54	3.55	-0.01
mjk008	90.70	0.1159	0.10	2.93	2.89	0.04
mjk020	90.40	0.0100	0.47	4.46	4.69	-0.23
mjk085	64.20	0.0975	0.48	5.04	5.04	0.00
mjk106	76.30	0.1100	0.10	2.93	3.36	-0.43
mjk107	119.90	0.1199	0.12	2.52	2.03	0.49
mjk108	78.10	0.1061	0.10	3.03	3.32	-0.29
mjk109	92.70	0.1104	0.10	3.00	2.85	0.15
mjk110	108.80	0.1120	0.10	2.85	2.35	0.50
mjk111	78.10	0.1043	0.10	3.01	3.33	-0.32
mjk112	95.30	0.1061	0.10	3.02	2.80	0.22
mjk113	98.30	0.1028	0.10	5.38	2.72	2.66
mjk040	54.20	0.0927	0.45	5.07	5.28	-0.21
mjk042	72.00	0.0955	0.51	4.68	4.91	-0.23
mjk046	89.10	0.0978	0.57	4.05	4.57	-0.52
mjk048	106.80	0.0996	0.51	5.90	3.83	2.07
mjk114	130.10	0.1283	0.02	1.11	1.35	-0.24
mjk115	130.20	0.1290	0.02	1.11	1.34	-0.22
mjk116	144.80	0.1310	0.02	1.26	0.88	0.38
mjk117	145.10	0.1311	0.00	0.57	0.81	-0.24
mjk118	145.20	0.1315	0.00	0.57	0.80	-0.23
mjk119	160.00	0.1331	0.00	0.15	0.34	-0.19
mjk068	118.90	0.1212	0.00	0.05	1.66	-1.61
mjk120	149.40	0.1259	0.12	2.55	1.10	1.45
mjk121	164.00	0.1283	0.07	-0.16	0.47	-0.63
mjk122	115.00	0.1260	0.07	1.60	1.99	-0.39
mjk123	115.10	0.1264	0.07	1.70	1.98	-0.28
mjk124	115.00	0.1270	0.07	1.43	1.98	-0.55
mjk125	117.10	0.1241	0.07	1.67	1.93	-0.26
mjk126	132.70	0.1259	0.07	1.46	1.45	0.01
mjk127	127.50	0.1269	0.07	1.86	1.60	0.26
mjk129	176.10	0.1339	0.07	0.05	0.07	-0.02

TABLE 12. LSER for Konnemann's Fish Toxicity

ID Number	V_{mc}	π_1	β	LOG Kow Observed	LOG Kow Predicted	Residual
mjk54	84.60	0.5900	0.10	2.91	3.05	-0.14
mjk59	101.80	0.5400	0.11	2.69	2.54	0.15
mjk63	99.80	0.6500	0.07	2.84	2.47	0.37
mjk104	115.10	0.3900	0.04	1.60	1.89	-0.29
mjk105	60.50	0.6200	0.00	3.54	3.49	0.05
mjk008	90.70	0.0800	0.10	2.93	2.86	0.07
mjk020	90.40	0.2700	0.47	4.46	4.08	0.38
mjk085	64.20	0.7100	0.48	5.04	4.94	0.10
mjk106	76.30	0.3800	0.10	2.93	3.31	-0.38
mjk107	119.90	0.0300	0.12	2.52	2.00	0.52
mjk108	78.10	0.6100	0.10	3.03	3.26	-0.23
mjk109	2.70	0.2900	0.10	3.00	2.80	0.20
mjk110	108.80	0.7500	0.10	2.85	2.29	0.56
mjk111	78.10	0.4000	0.10	3.01	3.26	-0.25
mjk112	95.30	0.3900	0.10	3.02	2.72	0.30
mjk113	98.30	0.3900	0.10	5.38	2.62	2.76
mjk040	54.20	0.4000	0.45	5.07	5.16	-0.09
mjk042	72.00	0.4000	0.51	4.68	4.79	-0.11
mjk046	89.10	0.4000	0.57	4.05	4.45	-0.40
mjk048	106.80	0.4000	0.51	5.90	3.70	2.20
mjk114	130.10	0.4000	0.02	1.11	1.35	-0.24
mjk115	130.20	0.4000	0.02	1.12	1.35	-0.23
mjk116	144.80	0.4000	0.02	1.26	0.89	0.37
mjk117	145.10	0.4000	0.00	0.57	0.82	-0.25
mjk118	145.20	0.4000	0.00	0.57	0.81	-0.24
mjk119	160.00	0.4000	0.00	0.15	0.34	-0.19
mjk068	118.90	0.4700	0.00	0.05	1.64	-1.59
mjk120	149.40	0.4700	0.12	2.55	1.07	1.48
mjk121	164.00	0.4000	0.07	-0.16	0.45	-0.61
mjk122	115.00	0.4000	0.07	1.60	1.99	-0.39
mjk123	115.10	0.4000	0.07	1.70	1.99	-0.29
mjk124	115.00	0.4000	0.07	1.43	1.99	-0.56
mjk125	117.10	0.4000	0.07	1.67	1.93	-0.26
mjk126	132.70	0.4000	0.07	1.46	1.44	0.02
mjk127	127.50	0.4000	0.07	1.86	1.60	0.26
mjk129	176.10	0.4000	0.07	0.05	0.07	-0.02

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